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Interfacial dislocations in TiN/GaN thin films

Ph Komninou†§, G P Dimitrakopulos†, G Nouet‡, Th Kehagias†, P Ruterana‡ and Th Karakostas†

† Department of Physics, Aristotle University of Thessaloniki, GR-54006 Thessaloniki, Greece
‡ ESCTM-CRISMAT, UMR 6508CNRS, ISMRA, 6 Boulevard Marechal Juin, 14050 Caen Cedex, France

E-mail: komnhnoy@auth.gr

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Abstract. Thin films of stoichiometric cubic TiN for ohmic contact formation are directly deposited, by rf magnetron sputtering at room temperature, on (0001) surfaces of GaN epilayers grown on *c*-plane sapphire. Chemical etching and *in situ* dry etching of the free GaN surface allows an epitaxial growth of the deposited TiN films as revealed by high resolution electron microscopy observations. Taking into account the experimentally determined orientation relationship of the two structures, (0001) GaN ∥ (111) TiN, $[11\bar{2}0]$ GaN ∥ $[1\bar{1}0]$ TiN, families of dislocations are expected in the interface plane to accommodate the misfit (∼5.8%) with a spacing of 4.5 nm. The mathematical formulation of the circuit mapping technique is used to analyse the misfit dislocation content on HREM images since it allows the exact determination of the Burgers vector. This gives a result $\frac{1}{2}[01\bar{1}]$ TiN or $\frac{1}{3}[1\bar{2}10]$ GaN. A demistep of height $c_{GaN}/2$ is observed at the TiN/GaN interface and from there a $(11\bar{2})$ twin emanates into the TiN layer. It appears that such demisteps have an important role in mediating the columnar growth of the TiN material.

1. Introduction

The defect content and interfacial structure of different materials used in thin film systems for the fabrication of optoelectronic devices and transistors affect their electrical characteristics. When epitaxial growth takes place the most effective mechanism to relieve the lattice mismatch between substrate and epilayer is the formation of misfit dislocations. The microstructure of such systems can be efficiently analysed by high resolution electron microscopy (HREM). In a previous paper we presented the electrical characteristics of TiN_x contacts deposited on both n- and p-type GaN. The results showed that the TiN contacts to n-type GaN were ohmic while they exhibited a rectifying behaviour on p-type GaN [1]. Investigation of the structure of this system has been already given elsewhere [2–4].

In this work we present an analysis of the defect structure of the TiN/GaN interface by means of HREM observations on specimens in cross-section. Misfit dislocations are characterized by the circuit mapping method, which allows the exact determination of their Burgers vector. Twinning in the TiN layer emanating from an interfacial demistep is also presented.

§ Corresponding author.

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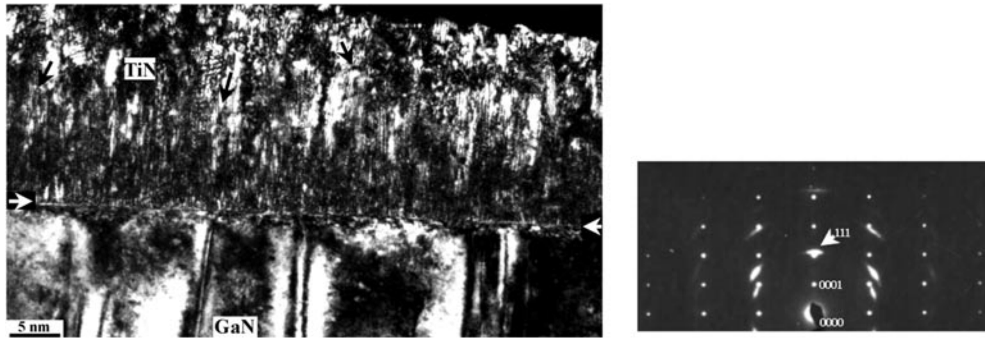


Figure 1. Conventional XTEM micrograph where the columnar growth of TiN thin film directly deposited on a flat (0001) GaN surface is visible. The corresponding diffraction pattern shows the orientation relationship of the two materials: the electron beam is along $[11\bar{2}0]$ GaN ∥ $[1\bar{1}0]$ TiN while the (0001) GaN lattice planes are parallel to the (111) TiN ones. Twinning in the TiN layers is depicted both by the twin spots in the diffraction pattern and the fringes visible in the micrograph and shown by the black arrows. White arrows indicate the GaN/TiN interface.

2. Experiment

TiN thin layers were directly deposited by dc reactive magnetron sputtering at room temperature on (0001) GaN films grown on *c*-plane sapphire. Details of the deposition conditions and the deposition system have been presented elsewhere [1, 5]. Cross-section transmission electron microscopy (XTEM) specimens were prepared using the conventional sandwich technique by mechanical grinding followed by ion milling. HREM observations were carried out on a TOPCON 002B electron microscope operated at 200 kV with a point to point resolution of 0.18 nm.

3. Results and discussion

In figure 1, a conventional XTEM micrograph, the columnar growth of TiN thin film directly deposited on a flat (0001) GaN surface is shown. From the corresponding diffraction pattern the orientation relationship of the two materials is determined. The $[11\bar{2}0]$ zone axis of GaN is parallel to $[1\bar{1}0]$ of TiN, both along the electron beam, while the (0001) GaN lattice planes are parallel to the (111) TiN ones. Twinning in the TiN layers is depicted both by the twin spots in the diffraction pattern and the fringes visible in the micrograph. Between neighbouring columns a small misorientation may exist, since the 111 reflection of TiN has an arc shape and a twin relation is also possible. The good quality of the deposited TiN layers and the epitaxial relationship of the two materials is shown in the diffraction pattern of figure 2, recorded from the specimen in plane view, i.e. along [0001] GaN ∥ [111] TiN. This epitaxial relationship is well known: $[11\bar{2}0]$ GaN ∥ $[1\bar{1}0]$ TiN, (0001) GaN ∥ (111) TiN, $(1\bar{1}00)$ GaN ∥ $(11\bar{2})$ TiN.

A network of three families of 60° misfit dislocations, with line directions along $\langle 11\bar{2}0\rangle$ GaN and $\langle 1\bar{1}0\rangle$ TiN, is expected in the interface in order to accommodate the 5.8% lattice mismatch. Along $\langle 1\bar{1}00\rangle$ GaN and $\langle 11\bar{2}\rangle$ TiN coincidence is achieved every $16d_{1\bar{1}00}$ GaN $= 17(3d_{22\bar{4}})$ TiN, where $d_{1\bar{1}00}$ and $d_{22\bar{4}}$ are the *d*-spacing of $(1\bar{1}00)$ and $(22\bar{4})$ planes of GaN and TiN respectively, leading to a 4.5 nm distance between them.

When the interface is imaged in cross-section with the electron beam being along $[11\bar{2}0]$ GaN ∥ $[1\bar{1}0]$ TiN, only one of the three families of misfit dislocations can be viewed edge on. Such a HREM micrograph is shown in figure 3(a), where the TiN/GaN interface is

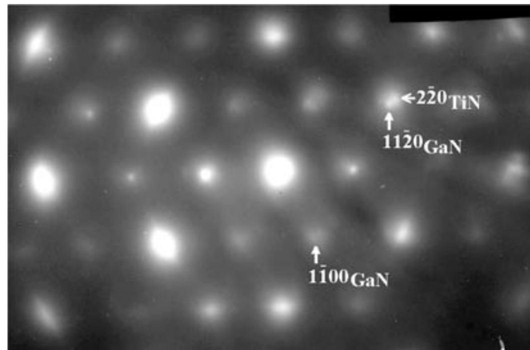
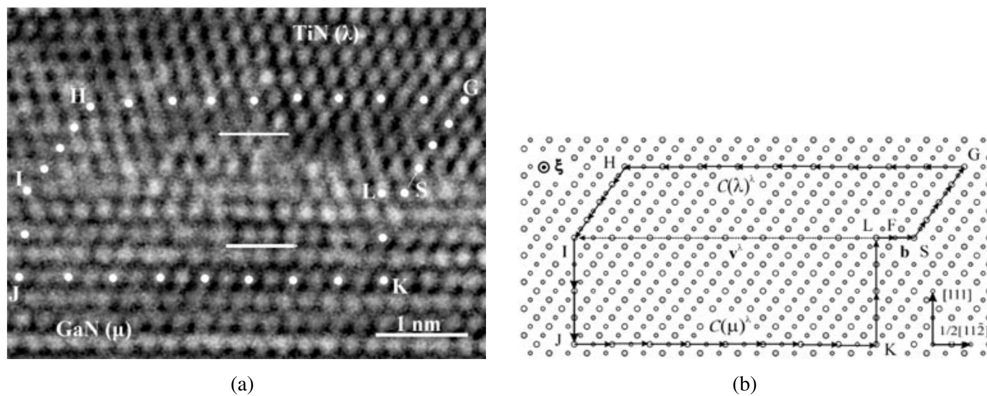


Figure 2. Diffraction pattern recorded in plane view showing the good quality of the deposited TiN layers and the epitaxial relationship of the two materials: electron beam along [0001] GaN ∥ [111] TiN, [11$\bar{2}$0] GaN ∥ [1$\bar{1}$0] TiN, (1$\bar{1}$00) GaN ∥ (11$\bar{2}$) TiN.



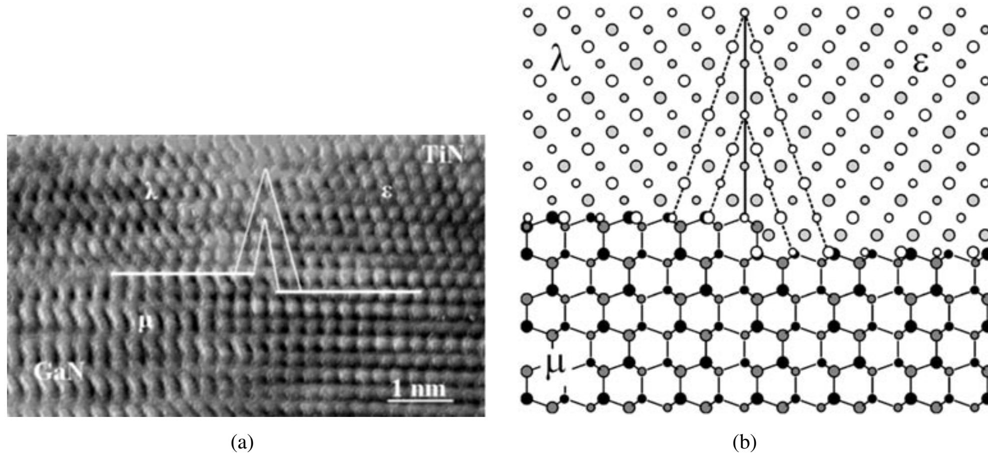
(a) (b)

Figure 3. (a) Cross-section HREM micrograph of the TiN/GaN interface, viewed along [11$\bar{2}$0] GaN ∥ [1$\bar{1}$0] TiN, indicating a closed right-handed circuit SGHIJKLS around a misfit dislocation. (b) Mapping of the closed circuit of (a) into the reference space (crystal λ). Closure failure $\boldsymbol{FS}$ arises. The probe vector $\boldsymbol{v}^\lambda$ is indicated. The line direction vector ξ of the defect is out of the page. (Open circles denote N atoms and grey circles Ti atoms. Large circles correspond to atoms at zero level, and small circles to atoms at height $a(2)^{1/2}/4$ respectively.)

clearly resolved containing one misfit dislocation. From image simulations the thickness of the specimen is estimated as 3.2 nm and the image was taken with a defocus −59 nm. Thus, each white dot corresponds to a projected atomic column.

In order to determine the Burgers vector we employ the circuit mapping method, which was originally introduced in a graphical form by Frank [6]. The method has been generalized by Pond and Hirth [7] under the mathematical framework of the *International Tables for Crystallography* [8].

In figure 3(a) a right-handed closed circuit, SGHIJKLS, is indicated around the misfit dislocation. An observer is imagined to make this excursion by undergoing a sequence of discrete symmetry operations [7], which, in our case, are translation operations. The circuit comprises a segment, SGHI, in the TiN crystal (designated as crystal λ) and a segment, IJKLS, in the GaN crystal (designated as crystal μ). We can describe each circuit segment mathematically and, for this purpose, we use Seitz operators as described in [8]. The operator



(a) (b)

Figure 4. (a) Cross-section HREM micrograph, recorded along $[11\bar{2}0]$ GaN ∥ $[1\bar{1}0]$ TiN, illustrating a demistep of height $c_{GaN}/2$ at the TiN/GaN interface, indicated by the white lines, and a $(11\bar{2})$ twin that emanates into the TiN layer. White lines on both sides of the twin boundary indicate the {111} atomic planes of the two twin-oriented crystallites. (b) Schematic illustration of a $(11\bar{2})$ twin boundary emanating from a GaN demistep. The interfaces on either side of the twin are energetically degenerate. (The projection is the same as in (a). Small circles are atoms at zero level, and large circles are atoms at height $a_{TiN}(2)^{1/2}/4$ in TiN and $a_{GaN}/2$ in GaN.)

corresponding to the λ circuit segment is expressed as

$$C(\lambda) = (\mathbf{I}, \boldsymbol{t}(\lambda)) = (\mathbf{I}, 4 \times \tfrac{1}{2}[\bar{1}\bar{1}0])(\mathbf{I}, 9 \times \tfrac{1}{2}[\bar{1}\bar{1}2])(\mathbf{I}, 4 \times \tfrac{1}{2}[110]) = (\mathbf{I}, 9 \times \tfrac{1}{2}[\bar{1}\bar{1}2]) \quad (1)$$

where the orthogonal part of the circuit operator that describes the orientation of the observer's frame at the end of the λ segment is equal to the identity, $\mathbf{I}$ (i.e. invariant orientation), and the translation part that describes the change in the observer's location is $\boldsymbol{t}(\lambda) = 9 \times \frac{1}{2}[\bar{1}\bar{1}2]$. Similarly, the operator corresponding to the μ segment is

$$\begin{aligned} C(\mu) &= (\mathbf{I}, -\boldsymbol{t}(\mu)) = (\mathbf{I}, \tfrac{1}{3}[2\bar{1}\bar{1}0])(\mathbf{I}, 2 \times [0001])(\mathbf{I}, 8 \times [1\bar{1}00])(\mathbf{I}, 2 \times [000\bar{1}]) \\ &= (\mathbf{I}, \tfrac{1}{3}[2\bar{1}\bar{1}0] + 8 \times [1\bar{1}00]). \end{aligned} \quad (2)$$

In order to obtain the Burgers vector, the two circuit segments are mapped in the appropriate bicrystalline reference space. As discussed in [7], for misfit dislocations, this reference space can be chosen to be the structure of one of the component crystals, and we choose the spacegroup of crystal λ (TiN) in this context. The circuit operator is then written as

$$C(\lambda\mu)^r = C(\mu)^r C(\lambda)^r \quad (3)$$

where the superscript r signifies that the circuit is mapped in the reference space. This mapping is illustrated graphically in figure 3(b); the circuit maps to SGHIJKLF in the reference space, and a closure failure $\boldsymbol{FS}$ arises. By substitution of the operators given in equations (1) and (2) in equation (3), we obtain

$$C(\lambda\mu)^\lambda = (\mathbf{I}, \boldsymbol{SF}) = (\mathbf{I}, \boldsymbol{t}(\lambda)^\lambda - \boldsymbol{t}(\mu)^\lambda). \quad (4)$$

In accordance with the RH/FS convention [7], the closure failure is given by $\{C(\lambda\mu)^\lambda\}^{-1} = (\mathbf{I}, \boldsymbol{FS}) = (\mathbf{I}, \boldsymbol{b}^\lambda)$, where $\boldsymbol{b}^\lambda$ is the Burgers vector expressed in the coordinate frame of crystal λ. As has been shown in [9], this reduces to the Frank–Bilby formulation [10]

$$\boldsymbol{b}^\lambda = (\mathbf{P}_\mu^{-1} - \mathbf{I})\boldsymbol{v}^\lambda \quad (5)$$

where $\mathbf{P}_\mu$ is the matrix describing the vector transformation by which the μ lattice is obtained from the λ one, and $\boldsymbol{v}^\lambda$ is the 'probe vector' lying along the interface (figure 3(b)). From equation (4) (or equivalently equation (5)) we obtain $\boldsymbol{b}^\lambda = \frac{1}{2}[01\bar{1}]$ or $\boldsymbol{b}^\mu = \frac{1}{3}[1\bar{2}10]$, identifying these defects as 60° dislocations. This vector is illustrated in figure 3(b). It is worth pointing out here the advantage of the mathematical formulation of circuit mapping over the graphical one, since it allows the exact determination of the Burgers vector, whereas the conventional Burgers circuit is based on a 2D projection of the bicrystal and hence gives only the apparent component of $\boldsymbol{b}$ that is perpendicular to the projection direction.

The epitaxial growth and twinning between two neighbouring crystallites are illustrated in the cross-section HREM micrograph of figure 4(a), viewed along $[11\bar{2}0]$ GaN ∥ $[1\bar{1}0]$ TiN. A demistep of height $c_{GaN}/2$ is observed at the TiN/GaN interface, indicated by the white lines, and from there a $(11\bar{2})$ twin emanates into the TiN layer. The white lines on both sides of the twin boundary indicate {111} atomic planes of the two twinned crystallites.

This configuration is explained if we consider that the $(11\bar{2})$ boundary compensates for the suppressed $\{10\bar{1}0\}$ mirror-glide symmetry of the GaN crystal, in accordance with Curie's principle of symmetry compensation [11] and it is illustrated schematically in figure 4(b). The $\{10\bar{1}0\}$ glide-mirror interrelates A to B type atoms in the . . . ABAB . . . stacking sequence of GaN. Hence the twin boundary emanates from a GaN demistep [12] of height $c_{GaN}/2$. The structures of the epitaxial interface on either side of the twin are crystallographically equivalent orientation variants, and hence they are energetically degenerate. The two twin-oriented TiN crystallites (designated λ and ε in figure 4(b)) and the GaN crystal (designated μ) constitute what has been termed a 'variant-constituted tricrystal'; a detailed account of such configurations has been given elsewhere [13], and it appears that they have an important role in mediating the columnar growth of the TiN material.

4. Conclusions

The columnar growth, the epitaxial relationship and twinning between neighbouring columns of stoichiometric cubic TiN thin film directly deposited by rf magnetron sputtering, at room temperature, on (0001) surfaces of GaN epilayers grown on c-plane sapphire for ohmic contact formation were studied by conventional cross-section and plane view transmission electron microscopy. Cross-section HREM observations revealed one of the three families of misfit dislocations that are expected in the interface plane to accommodate the misfit (∼5.8%) with a spacing of 4.5 nm. The mathematical formulation of the circuit mapping technique was used on HREM images for the determination of the Burgers vector. This gave a result of $\frac{1}{2}[01\bar{1}]$ TiN or $\frac{1}{3}[1\bar{2}10]$ GaN as expected. A demistep of height $c_{GaN}/2$ was observed at the TiN/GaN interface and from there a $(11\bar{2})$ twin to emanate into the TiN layer. The two twin-oriented TiN crystallites and the GaN crystal constitute a 'variant-constituted tricrystal'. Therefore it appears that such demisteps play an important role in mediating the columnar growth of the TiN film.

Acknowledgments

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References

[1] Dimitriadis C A, Karakostas Th, Logothetidis S, Kamarinos G, Brini J and Nouet G 1999 *Solid-State Electron.* **43** 1969

[2] Ruterana P, Nouet G, Kehagias Th, Komninou Ph, Karakostas Th, Di Forte Poisson M A, Huet F, Tordjman M and Morkoc H 1999 *Microscopy of Semiconducting Materials 1999 (Inst. Phys. Conf. Ser. 164)* ed A G Cullis and R Beanland (Bristol: Institute of Physics) p 567

[3] Ruterana P, Nouet G, Kehagias Th, Komninou Ph, Karakostas Th, Di Forte Poisson M A, Huet F and Morkoc H 1999 *Phys. Status Solidi* a **176** 767

[4] Ruterana P, Nouet G, Kehagias Th, Komninou Ph, Karakostas Th, Dimitriadis C A, Huet F and Di Forte Poisson M A 2000 *GaN and Related Alloys—1999 (Mater. Res. Soc. Symp. 595)* ed T H Myers *et al* (Warrendale, PA: Materials Research Society) p w11.75.1

[5] Logothetidis S and Alexandrou I 1995 *Appl. Phys. Lett.* **66** 502

[6] Frank F C 1951 *Phil. Mag.* **42** 809

[7] Pond R C and Hirth J P 1994 *Solid State Phys.* **47** 288

[8] Hahn T (ed) 1983 *International Tables for Crystallography* (Dordrecht: Reidel)

[9] Dimitrakopulos G P, Karakostas Th and Pond R C 1996 *Interface Sci.* **4** 129

[10] Christian J W 1981 *The Theory of Phase Transformations in Metals and Alloys* (New York: Pergamon) p 340

[11] Shubnikov A V and Koptsik V A 1974 *Symmetry in Science and Art* (New York: Plenum) p 334

[12] Pond R C 1989 *Dislocations in Solids* vol 8, ed F R N Nabarro (Amsterdam: North-Holland) p 1

[13] Dimitrakopulos G P and Karakostas Th 1996 *Acta Crystallogr.* A **52** 62